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Towards a Generic Multiscale Model for Boundary Lubrication

Hannes Holey[1), 2)*], Mohamed Tarek Elewa[1)], Andrea Codrignani[2)], Lars Pastewka[2)] and Peter Gumbsch[1)]

[1)]Institute for Applied Materials - Computational Materials Science, Karlsruhe Institute of Technology, Germany
[2)]Department of Microsystems Engineering, University of Freiburg, Germany
*Corresponding author: hannes.holey@kit.edu

The boundary lubrication regime is characterized by asperity contacts and lubricant films of only a few molecular diameter thickness. Due to the confinement and the accompanying relevance of fluid-wall interactions, the fluid behaves differently than in the bulk and common continuum models break down, because they do not consider molecular effects in the lubrication gap. Molecular dynamics simulations enable us to study these effects, but only on limited length and time scales. We here present a multiscale approach to model lubricated contacts using a coupled molecular - continuum scheme that overcomes these deficiencies.

Keywords: boundary lubrication, molecular dynamics, multiscale modeling

1. Introduction

Gap heights in lubricated contacts tend to decrease in industrial applications due to extreme operating conditions, the use of low viscosity lubricants, and environmental constraints regarding oil-based lubricants and additives. From a modeling perspective, this leads to challenges since classical continuum methods do not account for effects that occur on molecular length scales. Moreover, surface roughness leads to large variations of the fluid properties along lateral dimensions of the lubrication gap, which cannot be addressed by fixed-form constitutive relations. Our scheme uses Gaussian Process Regression to parametrize a generic constitutive relation based on non-equilibrium molecular dynamics (NEMD). Mass and momentum balance equations are solved on the macroscopic scale and determine boundary conditions for new NEMD runs if necessary. The scheme is similar to recent advances in modeling confined fluids [1].

2. Methods

2.1. Macroscopic model

We consider isothermal conditions for a compressible fluid, hence we solve a system of balance laws (Stokes equation)

$$\frac{\partial \boldsymbol{q}}{\partial t} = -\nabla \cdot \boldsymbol{f}, \qquad (1)$$

with the densities of conserved variables mass and momentum $\boldsymbol{q} = (\rho, \boldsymbol{j})^T$ and corresponding flux functions $f = (\boldsymbol{j}, p\boldsymbol{I} - \boldsymbol{\tau})^T$, where p denotes the pressure, $\boldsymbol{\tau}$ the viscous stress tensor and $\boldsymbol{I}$ the identity tensor. We obtain a two-dimensional description by averaging Eq. (1) over the gap height. The averaging procedure introduces a source term that contains both averaged and local flux components (at the walls) as well as the gap height function $h(x,y)$ and its gradient and therefore implicitly models the fluid-wall boundary condition. We solve the system using an explicit time-marching scheme and a two-dimensional finite volume discretization, where we use MacCormack's numerical flux approximation [2].

2.2. Microscopic model

We perform molecular dynamics simulations of a pressurized slab geometry with sliding walls at constant temperature. Since periodic boundary conditions cannot support a pressure gradient in lateral dimensions, we attach a "pump region" to the MD boxes and control the pressure-driven flow by fixing the mass flux in this region. The averaged stress components are measured far from the pump region and serve as training data for the parametrization of a dynamic constitutive relation.

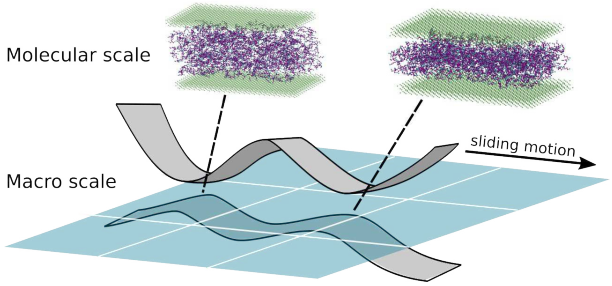

Figure 1: Schematic representation of the coupled molecular dynamics (MD) - finite volume scheme for a sliding contact.

3. Results

We test the coupled scheme for simple fluids in the hydrodynamics regime on periodic geometries and prove its validity by comparing it to continuum solutions based on the compressible Reynolds equation. The scheme is then applied in systems where continuum assumptions usually break down.

4. Discussion

The presented scheme enables us to study complex lubrication systems on relevant length and timescales without the need of explicit constitutive laws.

5. References

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